

The Green Chemistry Expert System (GCES)

Abstract

The GCES has been developed by the Industrial Chemistry Branch (ICB) of the Office of Pollution Prevention and Toxics. The impetus for development of the system was ICB's desire to share its expertise in using Green Chemistry to prevent pollution. ICB's experience arises from review of thousands of new chemicals as well as collecting and disseminating information on hundreds of green chemistry technologies. By condensing this expertise into a computer program, it is now easily shared with those involved in or interested in chemical manufacturing processes. In doing so, we hope to encourage chemists to identify hazardous chemicals in their processes and then find ways to reduce or eliminate their production or use.

The GCES is a stand-alone system that has been developed for free distribution. The system is both a computational and a database tool. It is designed to assess pollution prevention opportunities for specific chemical manufacturing processes and provide information on potential alternatives. While the system was originally designed with new chemicals review in mind, its analyses can be applied to existing chemicals just as easily. The present version is an initial release and the data available in the system to assist in the identification of greener alternatives will be significantly expanded in the next version.

The GCES has five modules: the SMART module, which stands for Synthetic Methodology Assessment for Reduction Techniques, Green Synthetic Reactions, Designing Safer Chemicals, Green Solvents/Reaction Conditions, and Green Chemistry References.

- ◆ The SMART module calculates the waste generated by a manufacturing process based on user input, categorizes that waste into hazard tiers, and prioritizes waste minimization based on the quantity and hazard of that waste. It is the first step in identifying opportunities for pollution prevention in a manufacturing process. It refers the user to the other GCES modules as appropriate for the reaction.
- ◆ The Green Synthetic Reactions module is a database of reactions that may be useful in identifying a way to make the same or similar product with less hazardous feedstocks or with less hazardous byproducts.
- ◆ The Designing Safer Chemicals module contains information on how to redesign a chemical product to reduce its hazard to human health or the environment. It also has a database of examples of products designed to minimize hazard.

- ◆ The Green Solvents/Reaction Conditions module contains information that may be helpful identifying an alternative to a hazardous solvent. It also contains reviews of recent green solvent advances and a database of examples of green solvent technology.
- ◆ The Green Chemistry Reference module is a database of hundreds of references from books, symposia, journals, and magazines, many with abstracts. It can be searched by category and sub-category or with a simple text search.

The current version of the Green Chemistry Expert System is available from the Green Chemistry web site at <http://www.epa.gov/greenchemistry>.